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a higher Fidelity Approval for Bulk  
Chemical Lethality Calculations  
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<h2 style="margin: 0;">A Higher Fidelity Approach for Bulk Chemical Lethality Calculations (U)</h2> <p style="margin: 10px 0;">Dr. Martin B. Richardson Mr. Kevin W. Bruening Ms. Erica M. Gomez MEVATEC Corporation</p> <p style="margin: 10px 0;">presented at The 9th Annual AIAA/BMDO Technology Conference U.S. Grant Hotel, San Diego, CA 17 - 20 July 2000</p> <div style="border: 1px solid black; padding: 2px; width: fit-content; margin: 0 auto;"> <small>Distribution Statement A: Approved for public release; distribution is unlimited.</small> </div>		
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### Abstract

The goal of bulk chemical lethality predictions is to determine potential casualties from the dissemination of a chemical payload under both offensive laydown and defensive engagement scenarios. While these two scenarios can involve radically different initial conditions in terms of altitude of release, amount of agent ejected, and the shape and droplet distribution of the agent cloud, they both rely upon atmospheric transport codes to track the agent cloud to the ground. All atmospheric transport codes require an initial description of the agent cloud (the source term) that consists of both the geometry of the agent cloud and the droplet distribution. In order to keep track of agent reaching the ground, a gridded array is often employed. The amount of agent that lands within any particular grid cell is generally recorded as the sum of the droplet masses. Owing to this summation process, information regarding the numbers and locations of individual droplets is lost, and further calculations using deposition values rely on a uniformly smooth distribution of agent (within a given cell). This implicit smoothing function is valid as long as the agent is deposited as a dense rain or mist such that individual droplet impacts make a negligible contribution to the overall amount of agent that gets deposited on a person. However, when the droplet distribution consists of larger, widely separated droplets, then the lethality calculations based upon a uniform distribution of agent can result in predictions that are inconsistent with a higher fidelity treatment of the actual distribution. In general, it can be shown that low average mean deposition levels underestimate casualties and high average mean deposition values overestimate casualties. The differences can be substantial.

In order to more accurately predict casualty calculations, a discrete droplet lethality methodology is currently being implemented into the BMDO lethality model PEGEM. This presentation will discuss the discrete droplet lethality methodology and present results of calculations demonstrating the importance of accounting for discrete droplet distributions.


<b>MEVATEC</b>	UNCLASSIFIED	
<b>Introduction (U)</b>		
<ul style="list-style-type: none"><li>• Casualty predictions for bulk chemical payload releases have traditionally been performed using aggregate values of agent uniformly spread out over a grid cell.<ul style="list-style-type: none"><li>– Mass of agent for every size bin contained within a given grid cell are summed together.</li><li>– The mean dose (total mass divided by grid cell area) is used for subsequent casualty calculations.</li></ul></li></ul>		
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The method generally employed for calculating casualties from a rain of bulk chemical agent is based upon summing the agent drop masses that landed within a grid cell and employing the mean concentration value (total agent mass divided by cell area) for defining the dose that each person receives.

<b>MEVATEC</b>	<p>UNCLASSIFIED</p> <h2>Introduction (U)</h2> 
<ul style="list-style-type: none"><li>• Employing such uniformly-distributed deposition values will <u>not</u>, in general, accurately reflect the actual doses of agent that a given population would receive from persistent agent delivered as a rain of droplets.</li><li>• Statistical variability produces a range of doses even for a mono-disperse distribution of drops.</li></ul>	
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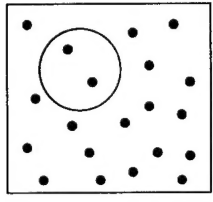
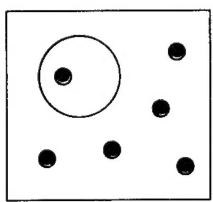
Use of uniformly-distributed agent will not, in general, properly account for the random effects of a discrete droplet distribution, owing to the statistical variability and thus range of doses a given population could receive.

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## Droplet Size and Dose (U)

- For low mean levels of agent deposited in large drops, mean separation distances can be in meters.
- All else being equal, the smaller the droplet size the greater the chance of getting hit, but the smaller the dose.
- Thus the **dose** a person could get from a specified average deposition value is **dependent on droplet size**.




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For a given mean level of agent, the dose that an individual could receive is a function of the droplet size. The smaller the droplets, the greater the chance of getting hit, but the smaller the dose.

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Implications (U)




- Accounting for discrete droplet effects on lethality calculations results in
  - **Greater** number of casualties at **low** lethal dose levels
  - **Fewer** number of casualties at **high** lethal dose levels

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A higher fidelity estimate of casualty calculations that accounts for the statistical drop distribution will tend to predict greater casualties in the regions where there is a low mean levels of agent and fewer casualties where there is a high mean level of agent.

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## Incorporating Droplet Distribution Effects into Lethality Calculations (U)



- A Statistical Casualty Model is being incorporated into the BMDO Post-Engagement Ground Effects Model  to determine the **dose distribution** in every grid cell with a non-zero population.
- The dose distribution, in turn, is used to calculate potential casualties.


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The BMDO Post-Engagement Ground Effects Model (PEGEM) version 3.6 is being upgraded to include a Statistical Casualty Model for bulk chemical agents.

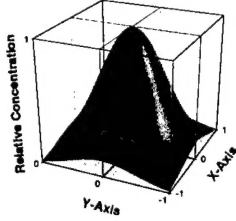
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**MEVATEC** **Statistical Casualty Model Basis (U)**

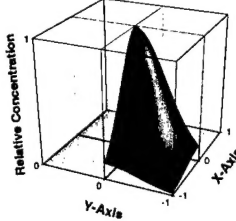


- The Statistical Casualty Model assumes a random distribution of drops and population.
- The number of drops within a grid cell (per size bin) is calculated from the mass fraction of the Gaussian-distributed mass concentration lying within that cell.

Full Gaussian Puff Covering 4 Grid Cells



Fraction of Gaussian Puff in 1 Grid Cell



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The Statistical Casualty Model assumes a random distribution of both drops and population. The number of drops for each drop size in a grid cell is calculated from the mass of agent in the grid cell associated with that drop size. A separate calculation is required to determine the mass associated with a given drop size by integrating over the fraction of the collapsed Gaussian puff for that drop size located within that grid cell.



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**MEVATEC** **Statistical Casualty Model Basis (U)**




- A Poisson distribution is used to quantify the number of drops each individual receives.
- Casualties are determined by summing the results of probit calculations over the calculated dose distribution in each grid cell.


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Owing to the small area of a person compared to the size of a grid cell, the likelihood of an individual getting hit by any particular drop is small. Under this condition, Poisson statistics are applicable. Once the dose distribution for the population within the grid cell is performed, casualty calculations are performed on that dose distribution using standard probit methodology.

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**Expected Number of Drops  
Impacting a Person (U)**



- If the number of drops in a given drop size bin  $i$  falling in a particular grid cell is  $n_i$ , then the number of those drops  $n_{hit,i}$  expected to strike a person is

$$n_{hit,i} = n_i \frac{A_p}{A_c} = n_i p$$

where  $A_p$  is the “exposed” area of a person and  $A_c$  is the area of a grid cell.


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The expected number of drops hitting a person is given by the number of drops falling within a grid cell times the area of a person exposed to the agent divided by the grid cell area.

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## Poisson Distribution (U)

- The probability of a person getting hit with various numbers of drops  $x$ , given the (low) probability of being hit by a single drop, can be expressed through the Poisson distribution



$$P(x) = \frac{e^{-\theta} \theta^x}{x!}$$

where  $\theta = np$  is the expected value.

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Definition of the Poisson distribution.


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	<b>Algorithm Summary (U)</b>	
<ul style="list-style-type: none"><li>• Calculate number of drops per size bin per grid cell.</li><li>• Calculate the expected value <math>np</math> for each drop size within the grid cell.</li><li>• Determine whether the value of <math>np</math> requires the <b>Poisson distribution</b> or if the mean level of agent is adequate.</li><li>• Independently assign drops (or, where applicable, mean values) from each size bin to each individual in a grid cell, resulting in a <b>dose distribution</b> for that cell.</li><li>• Employ a probit analysis on the dose distribution to determine casualties.</li></ul>		
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Summary of the steps used in the statistical casualty algorithm.

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Examples (U)



- The following examples compare results calculated using the statistical methodology with the mean dose per grid cell methodology.

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A comparison of casualty calculations between the mean agent methodology and the statistical methodology will be presented.

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Casualty Methodology  
Comparison (U)

The logo of the Missile Defense Agency, featuring a shield with a missile and the text "MISSILE DEFENSE AGENCY" and "DEPARTMENT OF DEFENSE".

TBM Bulk Chemical Payload Release

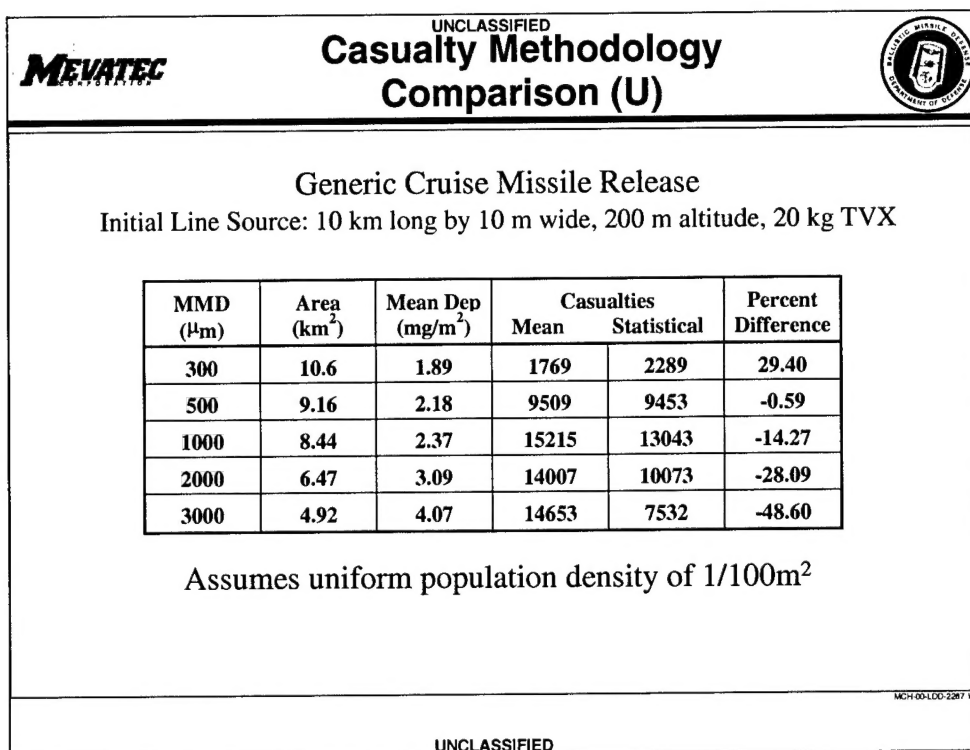
MMD (μm)	Altitude (km)	Payload Mass (kg)	Casualties Mean	Casualties Statistical	Percent Difference
1000	34	100	9753	31737	225
1000	34	50	231	10855	4600
500	20	100	85	4388	5060
500	20	50	0	1089	--
300	10	100	0	225	--
300	10	50	0	61	--

Assumes uniform population density of 1/100m<sup>2</sup>


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Casualty comparison examples are presented for three MMDs (1000, 500, and 300 μm), three altitudes (34, 20, and 10 km), and two payload masses (100 and 50 kg) that are indicative of post-engagement parameters following a HTK impact. Casualties are based upon a casualty area metric, i.e., uniform population with a density of 1/100m<sup>2</sup>. Differences in casualties between the mean and statistical methodologies can be significant, highlighting the need to account for the droplet distribution on casualty calculations. As can be seen in the table, there are some scenarios in which the mean methodology predicts no casualties -- in contrast to a small but potentially significant number using the statistical methodology.



Casualty comparison examples for a generic cruise missile release at 200 m above ground level are shown for 5 different MMDs, ranging from 300  $\mu\text{m}$  to 3000  $\mu\text{m}$ . For low mean deposition levels (300  $\mu\text{m}$  case), the mean methodology tends to underpredict relative to the statistical casualty model, whereas for higher mean deposition levels, the mean methodology tends to overpredict. In addition, the effects of an agent-rich "overkill" situation are clearly shown with the decreasing total number of casualties for MMDs greater than 1000  $\mu\text{m}$ .

<b>MEVATEC</b>	UNCLASSIFIED <b>Conclusion (U)</b>	
<ul style="list-style-type: none"><li>• Accounting for discrete droplet effects on lethality calculations results in a <b>more accurate assessment of casualties at both low and high lethal dose levels.</b></li><li>• Method to incorporate discrete droplet effects has been developed for PEGEM.</li></ul>		
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A method for accounting for the statistical nature of agent deposition on lethality calculations has been developed and is being incorporated into PEGEM.